

Density Matrix in Quantum Mechanics and Distinctness of Ensembles Having the Same Compressed Density Matrix

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We clarify different definitions of the density matrix by proposing the use of different names, the full density matrix for a single-closed quantum system, the compressed density matrix for the averaged single molecule state from an ensemble of molecules, and the reduced density matrix for a part of an entangled quantum system, respectively. We show that ensembles with the same compressed density matrix can be physically distinguished by observing fluctuations of various observables. This is in contrast to a general belief that ensembles with the same compressed density matrix are identical. Explicit expression for the fluctuation of an observable in a specified ensemble is given. We have discussed the nature of nuclear magnetic resonance quantum computing. We show that the conclusion that there is no quantum entanglement in the current nuclear magnetic resonance quantum computing experiment is based on the unjustified belief that ensembles having the same compressed density matrix are identical physically. Related issues in quantum communication are also discussed.

Keywords: full density matrix, compressed density matrix, reduced density matrix, distinction of ensembles

1. INTRODUCTION

1. In a quantum system, the wave function specifies all the physical properties of the system. The wave function provides the maximal information. A system with a wave function description is said to be in a pure state. In contrast sometimes there is incomplete information about a quantum system and this may be more common. Von Neumann and Landau proposed to use the density matrix to describe the state of a quantum system in this situation[1, 2]. It has been widely used nowadays, and is presented in standard textbooks and monographs on quantum mechanics, for instance in Refs. [3, 4, 5, 6, 7]. With the development of quantum information in recent years, there have been renewed interests in the density matrix formalism. It is the basic tool for the study of quantum entanglement, channel capacity in quantum communication and so on.
2. Though the density matrix has been proposed for nearly 80 years, there are still confusions and sometime disputes on matters related to it. Some are caused by a confusion in the terminology, but others are true disputes of the fundamental nature. A notable example is the question of distinctness of ensembles having the same density matrix. These matters are becoming more acute with the progress in quantum computation research and to cause true concerns. Whether current liquid nuclear magnetic resonance (NMR) quantum computation is genuine quantum mechanical or just a classical simulation is just one such problem.
3. In this article, we shall carefully inspect the definition of the density matrix, and that of the mixed state. This will remove a large number of disagreements. We propose to use three different terminologies for the density matrix in different situations: the full density matrix to describe the state of a single, closed quantum system, it always describes a pure state and is equivalent to the wave function; a reduced density matrix for the state of part of a coupled quantum system, it usually describes a mixed state; a compressed density matrix for an ensemble of independent quantum systems. After the classification of the density matrix, we will examine the distinctness of ensembles having the same compressed density matrix. We will show that ensembles having the same compressed density matrix can be distinguished physically. We show that this does not contradict one of the fundamental postulates of quantum mechanics that the density matrix completely specifies all the properties of a quantum ensemble, as stated by Asher Peres[8]. We then apply this result to the question of the nature of current NMR quantum computation, and show that the conclusion that there is no entanglement in the current NMR quantum computing is based on the unjustified belief that ensembles having the same compressed density matrix are physically identical, and hence is invalid. The implication of this result in quantum key distribution

and other areas of quantum information are also discussed.

2. DENSITY MATRIX AND MIXED STATE

4. First we introduce some notations in order to avoid confusion because different people use different definitions.

A molecule in this article refers to a single quantum system such as a qubit, a composite quantum system and so on.

An ensemble in this article is defined as a collection of N non-interacting molecules of the same kind in the same or different quantum states. An ensemble contains N non-interacting molecules, and there are N_i number of molecules in state $|\psi_i\rangle$, $i = 1, \dots, k$, $\sum_{i=1}^k N_i = N$.

This definition of an ensemble has been used by Shankar, Merzbacher, d’Espagnat, Von Neumann[5, 9, 10, 11]. A molecule is a quantum system which may contain a complex internal structure, for instance an atom, a molecule, a Bose-Einstein condensate all may be viewed as a molecule in an ensemble. The molecules are of the same kind, but they are independent of each other and can be distinguished, for example by their position, hence they are not identical particles. Usually they are far apart, so that their de Broglie waves rarely overlap. We note that the definition of ensemble by Asher Peres is different from ours [3]. In his definition, an ensemble is defined by a probability distribution and there are infinite number of molecules in an ensemble.

It is important to perceive the differences in the definition of ensemble in statistical physics and quantum mechanics. In statistical mechanics [12], an ensemble is a collection of infinite number of the system under identical physical constraints. For instance, a micro-canonical ensemble is specified by the particle number N and the total energy E . Then a system with N_i number of molecules in state $|\psi_i\rangle$, and $N = N_1 + N_2 + \dots + N_i + \dots$ satisfying the given constraints on the particle number and total energy will be a member in the statistical ensemble. Whereas in quantum mechanics, the system of N molecules itself is now an ensemble, each molecule is treated as a system and the density matrix ρ describes the state of averaged molecule in this system. This different comprehension of ensembles in statistical mechanics and quantum mechanics causes many of the misunderstanding.

A coupled quantum system is a quantum system with several constituents. For instance, a molecule is a coupled quantum system, and each atom in a multi-atom molecule is a constituent. The constituents in a

coupled quantum system may be confined, for instance the atoms in a molecule, or far away apart, for instance two entangled photon pairs forming a coupled quantum system.

By a sampling measurement of observable Ω , we mean the following. We select randomly one molecule from an ensemble and makes an Ω measurement on this molecule. Then the ensemble is restored to its original state, namely N_i molecules in state $|\psi_i\rangle$, and we randomly select a molecule again and makes an Ω measurement on the molecule. We repeat this process sufficient number of times. Then the result of the sampling measurement of Ω is the averaged value of these individual measurements, and it is denoted by $\langle\Omega\rangle$. In the density matrix formalism, the expectation value of an observable Ω in an ensemble, $\langle\Omega\rangle = \text{Tr}(\rho\Omega)$, should be understood in this way.

In contrast, **by a global measurement of observable Ω** , we mean a measurement on the whole ensemble: we fetch every molecule in the ensemble and measure its Ω . The result of the global measurement of Ω will be the sum of all these individual measurements. The fluctuation of the global measurement of Ω is understood in the same way as that for a quantum system: one prepares many copies of the same ensemble, he makes global measurement of Ω on each of these ensembles. The expectation value of the global measurement will be the averaged value of these global measurements, and the fluctuation is the standard deviation from this averaged (or mean) global measurement. We denote the global measurement by a subscript E . The expectation value of a global measurement of Ω is denoted by $\langle\Omega\rangle_E$. For instance, for an ensemble of nuclear spins, the z -component of the spin operator Σ_z for the whole ensemble is the sum of all the individual nuclear spins,

$$\Sigma_z = \sum_{i=1}^N \sigma_z(i).$$

One can obtain its value by measuring the total magnetic polarization of the whole ensemble, thus sometimes one can get the global measurement result without measuring each of the individual molecule.

The expectation value of a global measurement and the sampling measurement is related by the following

$$\langle\Omega\rangle_E = N\langle\Omega\rangle, \tag{1}$$

where N is the number of molecules in the ensemble.

5. Von Neumann defined a density matrix and mixed and pure states in the following way[11]. Consider the case in which one does not know what state is actually present in a system, for example when several states $|\phi_1\rangle, |\phi_2\rangle, \dots$ with respective probabilities w_1, w_2, \dots , ($w_1 \geq 0, w_2 \geq 0, \dots, w_1 + w_2 + \dots = 1$) constitute the description

of the system. Then the expectation value of a physical observable Ω in the system is

$$\langle \Omega \rangle = \sum_n w_n \langle \phi_n | \Omega | \phi_n \rangle = \text{Tr}(\rho \Omega). \quad (2)$$

The density operator, or density matrix

$$\rho = \sum_n w_n |\phi_n\rangle \langle \phi_n|, \quad (3)$$

is used to describe the state of the quantum system under study. It characterizes the mixture of states just described completely **with respect to its statistical properties**.

When only one w_i is equal to one and the rest w_i 's are zero, then the quantum system is described by a single wave function, and the system is said to be in a pure state. When more than one w_i 's are nonzero, the state is called a mixed state.

The above notion is commonly accepted. However, in practice there are different scenarios where the density matrix can be applied. For example, the abstract definition of density matrix is applied to an ensemble with N molecules. If in an ensemble of N independent molecules, there are N_i molecules in state $|\psi_i\rangle$, then the ensemble is described by the following density matrix

$$\rho = \sum_{i=1}^m w_i |\psi_i\rangle \langle \psi_i|, \quad (4)$$

where $w_i = N_i/N$ and m is the number of possible single molecule wave functions in the ensemble.

Here the density matrix represents the "state" of an averaged molecule from this ensemble: a molecule in this ensemble has $w_i = N_i/N$ probability in state $|\psi_i\rangle$. w_i is the probability a molecule is in state $|\psi_i\rangle$ if one fetches a molecule from the ensemble randomly. If $m > 1$, the ensemble is said to be a mixed ensemble, or simply a mixed state. If $m = 1$, the ensemble is an ensemble in which all molecules are in the same state, and the ensemble is called a pure ensemble, or simply a pure state.

This definition of mixed state is widely adopted in textbooks and monographs of quantum mechanics, for example in Shankar[9], Merzbacher [10] and so on. d'Espagnat has suggested to use the term, proper mixture for this type of object[5], and this practice is adopted in this article.

This definition of mixed state is also used by Asher Peres [3] and Preskill[4]. For example, in one of Peres's example, there are two different ensembles that have the same density matrix $\rho = \frac{1}{2}\mathbf{1}_2$, where \mathbf{I}_2 is a 2 by 2 unit matrix. One ensemble is prepared by preparing each qubit in either state $|0\rangle$ or $|1\rangle$ according to the result of a

coin-tossing. The other ensemble is prepared by making the state of each qubit in either

$$|\pm\rangle = (|0\rangle \pm |1\rangle)/2, \quad (5)$$

also according to the result of a coin-tossing. Though each individual qubit from both ensembles is in a definite quantum state, but **on average**, a qubit from the first ensemble has half probability in state $|0\rangle$ and $|1\rangle$ respectively, namely if one fetches a qubit from the prepared ensemble, there is half probability the qubit is in state $|0\rangle$ and another half probability in state $|1\rangle$. Similar statement could also be made for the second ensemble. One should note that in Peres's example, the ensemble is defined to have infinite number of molecules. In this article, we talk of ensembles with a finite number of molecules.

6. Landau proposed the density matrix in a different way [2]. In a paper on damping problems in quantum mechanics, Landau introduced the density matrix to study coupled quantum systems. Suppose there are two systems, A and B, coupled together. The wave function for the coupled AB-system is

$$|\psi_{AB}\rangle = \sum_{n,r} c_{nr} |\psi_n\rangle |\psi'_r\rangle. \quad (6)$$

The expectation value of an observable Ω pertinent to the A-system in this state is

$$\langle \Omega^A \rangle = \langle \psi_{AB} | \Omega^A | \psi_{AB} \rangle = \sum_{n,m} \rho_{A,nm} \Omega_{nm}^A = \text{Tr}(\rho_A \Omega^A), \quad (7)$$

where

$$\Omega_{nm}^A = \langle \psi_n | \Omega^A | \psi_m \rangle, \quad (8)$$

and

$$\rho_{A,nm} = \sum_r c_{nr}^* c_{mr} = \text{Tr}_B(|\psi_{AB}\rangle \langle \psi_{AB}|). \quad (9)$$

The density matrix ρ_A describes the "state" of the A-system. When the rank of the density matrix is greater than 1, the state is also a mixed state. This type of mixed state is different from the proper mixed state, although they have the same mathematical structure. d'Espagnat suggested to use the terminology, improper mixture, for this type of object. We also adopt this in this article.

7. There are two different situations that a probabilistic description is required. In one case, the description is due to our lack of information about the quantum system, but the quantum system itself is actually in a definite quantum state described by a wave function. For instance in quantum key distribution [13], Alice prepares a

sequence of qubits, each qubit is randomly prepared in one of the following states: $|0\rangle$, $|1\rangle$, $|+\rangle$, $|-\rangle$. To anyone other than Alice, each photon is in a proper mixed state described by $\rho = \frac{1}{2}\mathbf{I}_2$. But to Alice, it is in a definite pure state because she has prepared it herself.

In another situation, a probabilistic description is the best one can provide. Suppose that two qubits A and B are in a Bell-basis state,

$$|\phi_{AB}^+\rangle = \sqrt{\frac{1}{2}} \{|0_A 0_B\rangle + |1_A 1_B\rangle\}. \quad (10)$$

If one wants to describe the state of qubit A without mentioning qubit B , the best one can do is to use the density matrix $\rho_A = \frac{1}{2}\mathbf{I}_2$. If one measures the state of qubit there is half probability each to obtain $|0\rangle$ or $|1\rangle$. Anyone, without exception, will get this result. This is in contrast to the previous example in which Alice has full knowledge of each qubit.

8. There is an essential difference between the proper mixed state and the improper mixed state. In the proper mixed state, each individual molecule in an ensemble is in a definite quantum state. In an improper mixed state, the molecule is actually in such a state with the proposed probability distribution. In the example when qubits A and B are in a Bell-basis state, $|\phi_{AB}^+\rangle = (|0_A 0_B\rangle + |1_A 1_B\rangle)/\sqrt{2}$, the reduced density matrix for qubit A is $\rho_A = \frac{1}{2}\mathbf{I}_2$. In this state the qubit A is actually in state $|0\rangle$ and $|1\rangle$ **simultaneously**.
9. The mathematical formalism of the density matrix are well-known[6]. Its equation of motion in the Schoedinger picture obeys the Liouville equation

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho]. \quad (11)$$

The density matrix ρ is positively definite. Its properties are summarized as follows

$$\text{Tr}(\rho) = 1, \quad (12)$$

$$\rho^\dagger = \rho, \quad (13)$$

$$\text{Tr}(\rho^2) \leq 1. \quad (14)$$

It should be pointed out that wave function description can also be equivalently expressed in terms of a density matrix,

$$\rho = |\Psi\rangle\langle\Psi|. \quad (15)$$

The density matrix in this case of a pure state is characterized by the equality $\text{Tr}(\rho^2) = 1$. The density matrix with $\text{Tr}(\rho^2) < 1$ is a mixed state, either proper or improper.

3. THREE DIFFERENT DENSITY MATRICES AND MIXED STATES

3.1 The FULL DENSITY MATRIX for a single QUANTUM SYSTEM

10. The state of a single, closed quantum system is always described by a state vector $|\psi\rangle$. This is dictated by the basic postulate of quantum mechanics [9]: "the state of the particle is represented by a vector $|\psi(t)\rangle$ in a Hilbert space." The density matrix for such a system is $\rho = |\psi\rangle\langle\psi|$. In this case, the density matrix description and the wave function description are strictly equivalent, and the unphysical overall phase in the wave function description is naturally eliminated in the density matrix description. It contains **ALL** the physical information about the system. We call the density matrix in this case a **full density matrix**.

A single, closed quantum system may have complicated structures. For instance a Bose-Einstein condensate in an isolated environment is considered as a single closed quantum system. An isolated atom with many electrons and nucleons is another example. A quantum system of N 2-level molecules(or qubits) could also be viewed as a single quantum system if we want to describe all the details of the whole N qubits. The density matrix for such an N -qubits system is of $2^N \times 2^N$ dimension.

Though the state of such a system is always pure, a mixed state description for such a system is possible when one considers only the average properties of the system over a period of time, or over some parameters. For instance if the system is under rapid change in time and only average property of the system over a relatively long period of time is concerned, the state of the system could be described by a density matrix obtained by averaging over the time

$$\bar{\rho} = \int_{t_1}^{t_2} \lambda(t) \rho(t) dt, \quad (16)$$

where $\lambda(t)$ is some probability distribution function. If the resulting density matrix describes a mixed state, it is a proper mixed state because we have actually traded the space averaging in an ensemble with the time averaging for a single molecule over some time.

3.2 The COMPRESSED DENSITY MATRIX for an ENSEMBLE

11. We call the single-molecule density matrix over an ensemble of N independent molecules as a **compressed density matrix**. If the compressed density matrix is pure, it indicates that all the single molecules in the

ensemble are in the same quantum state. If the compressed density matrix is a mixed one, it represents an ensemble with molecules in distinct quantum states. As stressed earlier, each individual molecule in the ensemble is in a definite quantum state, rather than in different states with respective probabilities. A mixed state arising from the average over an ensemble is called a proper mixture by d’Espagnat[5] as we mentioned earlier. Mixed state from this average is called the ignorance interpretation by Cohen [14].

3.3 REDUCED DENSITY MATRIX in composite QUANTUM SYSTEM

12. The density matrix obtained by tracing out partial degrees of freedom of a coupled system is called **reduced density matrix**. Suppose there are M constituent molecules in a coupled quantum system. The wave function of the coupled system is $|\Psi_{A_1 A_2 \dots A_M}\rangle$. The reduced density matrix for molecule A_i can be obtained by tracing out the degrees of other molecules

$$\rho_{A_i} = \text{Tr}_{A_1 A_2 \dots A_{i-1} A_{i+1} \dots A_M} (|\Psi_{A_1 A_2 \dots A_M}\rangle \langle \Psi_{A_1 A_2 \dots A_M}|). \quad (17)$$

One can also define reduced density matrix for two or more molecules by tracing the degrees of freedom of the remaining molecules, for instance, the reduced density matrix for molecules A_i and A_j is defined as

$$\rho_{A_i A_j} = \text{Tr}_{A_1 A_2 \dots A_{i-1} A_{i+1} \dots A_{j-1} A_{j+1} \dots A_M} (|\Psi_{A_1 A_2 \dots A_M}\rangle \langle \Psi_{A_1 A_2 \dots A_M}|). \quad (18)$$

The reduced density matrix has also been defined for identical particle systems. For an M -identical-particle system, one can define one-particle, two-particle, ... reduced density matrices as follows [15]

$$\begin{aligned} \rho^{(1)} &= \text{Tr}_{i_2 i_3 \dots i_M} (\rho), \\ \rho^{(2)} &= \text{Tr}_{i_3 \dots i_M} (\rho), \\ &\vdots \\ \rho^{(M-1)} &= \text{Tr}_{i_M} (\rho), \end{aligned} \quad (19)$$

where ρ is the density matrix for the coupled M -particle system. The whole M -particle system is treated as a single quantum system. The subscript i_k is the single-particle state index. These definitions are useful in the study of quantum entanglement in identical particle systems[16, 17].

It is worth noting that an M -particle coupled quantum system is different from an ensemble of M independent molecules. Usually the particles in an M -particle coupled quantum system are interacting and correlated.

However the molecules in an ensemble described by a compressed density matrix are independent and non-interacting. The coupled M particle system should be described by a M -particle density matrix, while an ensemble of M molecules is described by a single molecule compressed density matrix. For example, a M -qubit system is described by a $2^M \times 2^M$ density matrix, and an ensemble of M qubits, such as M spin-1/2 molecules is described by a 2×2 density matrix. In an NMR ensemble of 7-qubit molecules, there are usually $N = O(10^{16})$ molecules. However the compressed density matrix for the ensemble is $2^7 \times 2^7$, rather than $2^{7N} \times 2^{7N}$ [18].

An improper mixed state usually could not be identified with a proper mixed state with the same density matrix[5], as we see they represent different objects though their mathematical descriptions are the same. This type of mixed state was interpreted by Cohen as the ancilla interpretation [14].

13. It is useful to make a comparison between a single qubit and a coupled 2-qubit system to demonstrate the difference between a pure quantum state and an improper mixed state. Suppose a single qubit A is in state

$$|+x_A\rangle = \sqrt{\frac{1}{2}}\{|0_A\rangle + |1_A\rangle\}. \quad (20)$$

Consider another system in which qubit A and qubit B form an entangled state

$$|\phi_{AB}^+\rangle = \sqrt{\frac{1}{2}}\{|0_A 0_B\rangle + |1_A 1_B\rangle\}. \quad (21)$$

If one measures σ_z on qubit A, he will obtain $|0_A\rangle$ and $|1_A\rangle$ with 50% probability in each case. But if he measures σ_x on qubit A, he will obtain with certainty $|+x_A\rangle$ in the first case as it is an measurement on an eigenstate, whereas he will still have 50% probability to obtain $|+x_A\rangle$ and $|-x_A\rangle$ respectively in the latter case.

4. THREE SIMPLE EXAMPLES

14. We study three ensembles of qubits, that will be all described by the same mathematical density matrix $\rho = \frac{1}{2}I_2$ when N approaches infinity, to illustrate the different mixed states and their relationship. Suppose there are N pairs of qubits in state given by Eq. (21). All the A qubits are given to Alice and all B qubits to Bob. They form ensembles A_1 and B_1 respectively. Hence each A qubit molecule in A_1 is in an improper mixed state described by reduced density matrix $\rho_A = \frac{1}{2}I_2$, and similarly each B qubit molecule in ensemble B_1 is also in an improper mixed state with the same reduced density matrix. It should be pointed out that all the A qubit molecules in ensemble A_1 are in the same state, there is no difference between the states of the different molecules in ensemble A_1 . The same conclusion can also be said about ensemble B_1 . If one looks at the compositions of the

ensembles, one could say that the ensembles are "pure", as they are made of molecules all in the same "state", though the "state" is not a pure quantum state described by a single state vector. This is a generalization of the usual pure state in which all the molecules are in the same quantum state described by a wave function.

In the second example, one performs σ_z measurement on each qubit in ensemble B_1 . Because of the collapse of state in quantum mechanics, each qubit in B_1 collapses into either $|0\rangle$ or $|1\rangle$, with equal probabilities. Consequently, the corresponding A molecules in ensemble A_1 also collapses into state $|1\rangle$ or $|0\rangle$ respectively. The ensembles after the measurement are called A_2 and B_2 respectively. In ensemble B_2 , each qubit is in a definite quantum state and the preparer of the ensemble who performs the σ_z measurement knows all these information. He also knows the state of A molecules in ensemble A_2 as he can infer from the prior entanglement between qubit A and B and the result of his measurement of qubit B . Suppose after the measurement, the number of qubits in state $|0\rangle$ (or $|1\rangle$) is $N/2 - N_\delta$ (or $N/2 + N_\delta$), then the compressed density matrix of A_2 is

$$\rho_{A_2} = \begin{pmatrix} \frac{1}{2} - \frac{N_\delta}{N} & 0 \\ 0 & \frac{1}{2} + \frac{N_\delta}{N} \end{pmatrix}. \quad (22)$$

When N approaches infinity, the compressed density matrices for qubit A_2 and B_2 all become $\rho = \frac{1}{2}\mathbf{I}_2$. N_δ is a random number, can be positive and negative or zero, and is proportional to \sqrt{N} according to statistics.

In the third example, one performs σ_x measurement on each qubit in ensemble B_1 . Again due to the collapse of state in quantum mechanics, each qubit in B_1 collapses into either $|+x\rangle$ or $|-x\rangle$, with equal probabilities. Consequently, the corresponding B molecules in ensemble A_1 also collapses into state $|-x\rangle$ or $|+x\rangle$ respectively. The ensembles after the measurement are called A_3 and B_3 respectively. In ensemble B_3 , each qubit is also in a definite quantum state and the preparer of the ensembles who has performed the σ_x measurement knows all these information. He also knows the state of A molecules in ensemble A_3 . Suppose after the measurement, the number of qubit in $|+x\rangle$ (or $|-x\rangle$) is $N/2 - N_x$ (or $N/2 + N_x$), then the compressed density matrix of A_3 is

$$\begin{aligned} \rho_{A_3} &= \left(\frac{1}{2} - \frac{N_x}{N} \right) | +x \rangle \langle +x | + \left(\frac{1}{2} + \frac{N_x}{N} \right) | -x \rangle \langle -x | \\ &= \begin{pmatrix} \frac{1}{2} & -\frac{N_x}{N} \\ -\frac{N_x}{N} & \frac{1}{2} \end{pmatrix}. \end{aligned} \quad (23)$$

Again the compressed density matrices for qubit A_3 and B_3 are all approaching $\rho = \frac{1}{2}\mathbf{I}_2$ when N approaches infinity. Here N_x is also random, could be positive, negative or zero, and is proportional to \sqrt{N} .

We stress here that when the number of qubit N is finite, the three ensembles are different and they are

distinguishable physically. When a measurement is performed on an ensemble, the compressed density matrix of the resulting ensemble is usually uncontrollable, and this is especially so when the number N is small. Even if one performs the measurement on the same observable, the resulting compressed density matrix is different at different times. Suppose one has N EPR pairs in state in Eq. (21). As usual, the A particles are given to Alice and the B particles given to Bob. When Bob performs σ_z measurement on each of his B particles, he will get an ensemble with a compressed density matrix ρ_B . Suppose he repeats the process a second time starting from state in Eq.(21), he will obtain another ensemble with a compressed density matrix ρ'_B . Usually $\rho_B \neq \rho'_B$ as can be seen in Eq.(22). An extreme case is an ensemble A_1 with $N = 2$. Before any measurement, the state of any of the two particles is an improper mixed state with density matrix, $\rho = 1/2I_2$. Suppose σ_z is measured on each of the two particles. Then four different results may occur: 1) both qubits have spins up, and the resulting compressed density matrix is a pure state,

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; \quad (24)$$

2) both qubits have spins down, and this gives a compressed density matrix,

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}; \quad (25)$$

3) one qubit has spin up and the other spin down, and vice versa. In both cases, the compressed density matrices of the resulting ensemble are

$$\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \quad (26)$$

This third case is more probable, and there is 50% probability to occur, whereas case 1 and 2 each has 25% probability to occur.

Though the three ensembles are distinguishable, they can not be exploited to realize faster-than-light quantum communication because one can not ascribe a unique compressed density matrix to a measurement because of the fluctuation in the quantum measurement. Impossibility of faster-than-light communication does not imply the indistinguishability of ensembles having the same compressed density matrix, which has been discussed recently.[19]

5. DISTINCTION OF ENSEMBLES HAVING THE SAME COMPRESSED DENSITY MATRIX

5.1 Present STATUS

15. Penrose doubts the completeness of the density matrix description. In an example where A (I myself) on Earth and B (my colleague) on the Moon each hold a particle from an EPR pair, Penrose states that "However, it is hard to take the position that the density matrix describes reality. The trouble is that I do not know that I might not, sometimes later, get a message from the Moon, telling me that my colleague actually measured the state and found the answer to be such and such. Then, I know what my particles's state must actually be. The density matrix did not tell me everything about the state of my particle. For that, I really need to know the actual state of the combined pair. So, the density matrix is sort of provisional description, and that is why it is sometimes called FAPP(i.e., for all practical purposes)." [21]

Here Penrose refers to what we call the reduced density matrix for a composite quantum system of two constituent particles. In our later discussion, we mainly focus our attention to the compressed density matrix.

16. It is commonly believed that ensembles with the same compressed density matrix are physically identical. We believe that this misbelief can largely be eliminated once a clear distinction between the compressed and the full density matrices is established.

A complexity arises due to the indistinction of proper mixed state and improper mixed state. Here we are talking about the distinction of ensembles with the same compressed density matrix rather than different composite systems with the same reduced density matrix. At present, there is intensive research work on quantum entanglement based on reduced density matrix for composite quantum systems. The distinction of ensembles having the same compressed density matrix we address here is not concerned with coupled quantum systems.

After clearing up those confusions in the terminology, there are still some authors who believe that ensembles with the same compressed density matrix are physically identical.

17. Asher Peres stresses that ensembles with infinite number of particles having the same compressed density matrix could not be distinguished physically. He uses an example to illustrate this idea. In one ensemble with infinite number of photons, each photon is prepared in either the $|H\rangle = |0\rangle$ state or $|V\rangle = |1\rangle$ state according to the result of coin-tossing. Hence the compressed density of this ensemble is $\rho = \frac{1}{2}1_2$. In another ensemble of infinite number of photons, each photon is prepared in the left-handed circular or right-hand circular state according

to the result of coin-tossing, and the compressed density matrix is also $\rho = \frac{1}{2}1_2$. Peres argued that there are no physical means to distinguish these two ensembles. He has elevated this into a fundamental postulate in quantum mechanics

The (compressed) ρ matrix specifies all the physical properties of a quantum ensemble (with infinite number of molecules).

Here the words inside the parenthesis are added by the authors to conform to the terminology used in this article.

At first sight, it may seem that this fundamental postulate excludes any possibility of distinguishing ensembles with the same compressed density matrix. However, it is not so because Peres' definition of ensemble is different from ours. Peres' ensemble contains an infinite number of molecules and it only exists conceptually as stressed by Peres[3]. Thus it does not exclude the possibility of distinguishing ensembles with a finite number of molecules having the same compressed density matrix.

In fact, Peres stated that finite particle number ensembles with the same compressed density matrix can be physically distinguished [20]. In this example, Peres constructed two ensembles with 1 million qubits each. In one case, half of the qubits are polarized in $|0\rangle$ state and the other half in state $|1\rangle$. In another case, half of the qubits are in state $\frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$ and the other half in state $\frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$. With high probability, people can distinguish the two ensembles (assemblies in Peres's term). The probability of failure is proportional to $\frac{1}{\sqrt{N}}$ where N is the number of molecules in the ensemble. Apparently, as N increases, the probability of failure is approaching zero.

18. Preskill stresses that differently prepared ensembles with the same compressed density matrix are not distinguishable on one hand, but he also points out different preparations of ensembles with the same compressed density matrix could be distinguished physically with some additional external help[4]. It is noted that Preskill's ensemble has a fixed number of molecules. Explicitly, Preskill proposed a method to distinguish the ensembles A_2 and A_3 in section 4. He presumably assumes that the compressed density matrix of A_2 and A_3 are the same, which is usually not true when the number of particles N is a fixed number. Suppose Bob starts from ensemble B_1 and makes a σ_x measurement on his B qubit molecules and hence prepares the ensemble B_3 and A_3 . Alice can find out what ensemble her ensemble is with some help from Bob: Bob tells Alice the result of the measurement for each B qubit molecule, whether up or down, but he does not tell her what measuring basis

he has used. Alice can choose any measuring basis, whether σ_x or σ_z , to measure each of her A qubit. If Alice chooses σ_x , her result will have perfect accordance with Bob's. If she chooses σ_z , only 50% of the results agree with Bob's. Hence Alice "does have a way to distinguish Bob's two preparation methods"[4].

19. d'Espagnat pointed out that ensembles having the same compressed density matrix can be distinguished physically by observing fluctuations of some observables. He has illustrated this in an ensemble of N qubits[5]. In ensemble S_1 , a half of qubits are in state $|0\rangle$ and another half are in state $|1\rangle$ where $|0\rangle$ and $|1\rangle$ are the eigenstates of operator σ_z , the Pauli matrix. In ensemble S_2 , a half of qubits are in state $|+x\rangle$ and another half are in states $|-x\rangle$ where $|+x\rangle$ and $|-x\rangle$ are the eigenstates of operator σ_x . In both ensembles, the compressed density matrix is $\rho = \frac{1}{2}1_2$. Although the average value of any observable Ω , in our terminology in a sampling measurement, for both ensembles are all expressed as

$$\langle\Omega\rangle = \text{Tr}(\rho\Omega), \quad (27)$$

the fluctuation of an observable will be different for ensembles with different compositions. Translated into our language, d'Espagnat actually refers to the fluctuation of a global measurement is different for different ensemble compositions with the same compressed density matrix. d'Espagnat used the following observable

$$\Sigma_z = \sum_{i=1}^N \sigma_z(i), \quad (28)$$

where the summation over i is made over all the molecules in the ensemble. For ensemble S_1 , the fluctuation of Σ_z is zero,

$$(\Delta\Sigma_z)_E = 0, \quad (29)$$

because each molecule is in an eigenstate of σ_z and every measurement of Σ_z on the whole ensemble will give identical result. However for ensemble S_2 , the fluctuation is

$$(\Delta\Sigma_z)_E = \sqrt{N}, \quad (30)$$

namely if one measures Σ_z on the whole ensemble, different result may be obtained at different times. By observing the fluctuation one can distinguish between the two ensembles with the same compressed density matrix.

5.2 ENSEMBLES with the same FULL DENSITY MATRIX are identical

20. Suppose one treats the whole ensemble having N molecules as a single quantum system, the ensemble is described by a full density matrix. If each molecule in the ensemble is independent and non-interacting, then the state of the ensemble is given by

$$|\psi_E\rangle = |\psi_1(1)\rangle|\psi_1(2)\rangle \cdots |\psi_1(N_1)\rangle|\psi_2(N_1 + 1)\rangle \cdots |\psi_2(N_1 + N_2)\rangle \cdots, \quad (31)$$

where the number inside the round bracket is the labelling of the molecule and the subscript refers to the state in which the molecule is in. The state $|\psi_E\rangle$ is the product of states of individual N molecules. The density matrix for the whole ensemble of N molecules is $\rho = |\psi_E\rangle\langle\psi_E|$. Since the wave function contains all the information about the system, the corresponding density matrix completely describes the state of the whole ensemble. We conclude that ensembles with the same full density matrix are physically identical. In this case, the density matrix is always one representing a pure state of a quantum system with N molecules. **If the full density matrices of the two ensembles are the same, then the two ensembles are physically identical.**

5.3 ENSEMBLES having the same COMPRESSED DENSITY MATRIX but with different PARTICLE NUMBERS are physically distinguishable

21. First, let's discuss the case of two ensembles having the same compressed density matrix but with different molecule numbers. With ideal measuring sensitivity, one can measure up to the accuracy of single molecule. Then from the expectation value of a global measurement alone, one can distinguish the two ensembles. The expectation of any observable with the form

$$\Omega = \sum_{i=1}^N \Omega(i), \quad (32)$$

will be sufficient to distinguish the two ensembles, because the expectation of observable Ω is

$$\langle\Omega\rangle_E = N\text{Tr}(\rho\Omega). \quad (33)$$

Because different molecule number N will give different expectation value, one can distinguish these ensembles from the expectation value directly. This is easy to understand if we compare two different amount of samples in nuclear magnetic resonance experiment. In NMR, the measured quantity is the total magnetization, and is equivalent to the signals in coil. The larger the sample, the stronger the measured signal.

5.4 General EXPRESSION for the FLUCTUATION of OBSERVABLES in GLOBAL MEASUREMENT

22. Generalizing the idea of d’Espagnat, ensembles having the same compressed density matrix could be distinguished by inspecting the fluctuation of some observables in global measurement. By this method, we can distinguish ensembles upto different physical composition: the number of molecules N_i in state $|\psi_i\rangle$.

Suppose there are N molecules in an ensemble with N_k molecules in state $|\psi_k\rangle$, and $k = 1, \dots, m$. The fluctuation of the observable

$$\Omega = \sum_{i=1}^N \Omega(i), \quad (34)$$

where i is the molecule index in the ensemble, is

$$(\Delta\Omega)_E = \sqrt{N(\text{Tr}(\Omega^2\rho) - \sum_k N_k \langle\psi_k|\Omega|\psi_k\rangle^2)}, \quad (35)$$

where the summation is over the possible single molecule states in the ensemble. It is apparent that the second term under the square-root is composition sensitive: ensembles with different compositions will give different results. This can be comprehended in the following way. For a single molecule in state $|\psi_k\rangle$, the fluctuation of Ω squared is

$$(\Delta\Omega)_k^2 = \langle\psi_k|\Omega^2|\psi_k\rangle - \langle\psi_k|\Omega|\psi_k\rangle^2, \quad (36)$$

and contribution from N_k such molecules is $N_k(\Delta\Omega)_k^2$, and the total contribution from all the molecules in the ensemble is $\sum_k N_k(\Delta\Omega)_k^2$. With some simple calculation, this gives the result in Eq. (35).

This result can be derived directly if one recalls that the state of the whole ensemble is Eq.(31) The fluctuation of observable Ω , namely the fluctuation of the global measurement is

$$(\Delta\Omega)_E = \sqrt{\langle\Psi_E|\Omega^2 - (\langle\Omega\rangle)_E^2|\Psi_E\rangle}. \quad (37)$$

The expression inside the square-root can be calculated and it is

$$\begin{aligned} & \langle\psi_E| \left(\sum_i \Omega(i)^2 + \sum_{i \neq j} \Omega(i)\Omega(j) - \sum_i \langle\psi_E|\Omega(i)|\psi_E\rangle^2 - \sum_{i \neq j} \langle\psi_E|\Omega(i)\Omega(j)|\psi_E\rangle \right) |\psi_E\rangle \\ &= \sum_k \langle\psi_k|\Omega^2|\psi_k\rangle - \sum_k N_k \langle\psi_k|\Omega|\psi_k\rangle^2, \end{aligned} \quad (38)$$

where i runs over the molecules in the ensemble and k runs over all possible single molecule states in the ensemble.

5.5 Composite QUANTUM SYSTEMS with the same REDUCED DENSITY MATRIX

23. Different composite quantum systems may produce the same reduced density matrix. They could be distinguished if one measures quantities involving the whole composite quantum system. For instance let us consider two systems of an EPR pair A and B , one in state

$$|\psi_{AB}^1\rangle = \sqrt{\frac{1}{2}} \{|0_A 0_B\rangle + |1_A 1_B\rangle\}, \quad (39)$$

and another in state

$$|\psi_{AB}^2\rangle = \sqrt{\frac{1}{2}} \{|0_A 0_B\rangle - |1_A 1_B\rangle\}. \quad (40)$$

In both cases, the reduced density matrix is $\rho_A = \frac{1}{2}1_2$. By measuring the observables of molecule A alone, one can not distinguish these two different composite quantum systems. However, the two systems will be distinguished the moment one makes a joint Bell-basis measurement.

6. THE NATURE OF ENSEMBLE NUCLEAR MAGNETIC RESONANCE QUANTUM COMPUTING

24. Ensembles with the same compressed density matrix can be distinguished physically is very important in quantum information processing. One important issue is the nature of room-temperature NMR quantum computing. It has been widely accepted that NMR quantum computing is not quantum mechanical because there is no entanglement in each step of the NMR quantum computing[22]. We point out here that this conclusion is based solely on the unjustified belief that ensembles having the same compressed density matrix are identical.

The major argument in Ref.[22] is to rewrite the effective density matrix, which is the compressed density matrix of the effective pure state obtained after the effective pure state technique,

$$\rho = \left(\frac{1-\epsilon}{4}\right) I_d + \epsilon \rho_{eff}, \quad (41)$$

where ρ_{eff} is the effective pure state density matrix, and ϵ is a number about 10^{-6} large and I_d is $d \times d$ unit matrix, into a convex decomposition of product-state density matrices,

$$\rho = \sum_i C_i \left(\rho_1 \otimes \cdots \rho_M \right)^i, \quad (42)$$

	P_1	P_2	P_3	P_4	P_5	P_6
P_1	ϵ		$-\epsilon$			
P_2		$-\epsilon$			ϵ	
P_3			ϵ			ϵ
P_4	$-\epsilon$			ϵ		
P_5		ϵ			$-\epsilon$	
P_6			$-\epsilon$			ϵ

TABLE I: C_{ij} for the effective pure Bell-state. A space means that coefficient is zero.

where C_i is the decomposition coefficient and $(\rho_1 \otimes \cdots \rho_M)^i$ is the density matrix representing the product of M qubits. This convex decomposition is possible when ϵ is small and the qubit number M is small. Since the product state does not have entanglement, then it was concluded by the equivalence of ensembles having the same compressed density matrix that the current NMR quantum computing does not have quantum entanglement, and hence is not genuine quantum mechanical.

From the previous discussions in this article, we see that the conclusion is based on an unjustified belief. Though the compressed density matrix of the effective pure state could be rewritten into convex decomposition of products state density matrices, they are not physically equivalent. As a simple example, we show that the effective Bell-state ensemble and its product state decomposition in Ref.[22] can be distinguished physically. The effective Bell-state compressed density matrix is

$$\rho = \frac{1-\epsilon}{4}I_4 + \epsilon\rho_{Bell}, \quad (43)$$

where $\rho_{bell} = (|00\rangle + |11\rangle)(\langle 00| + \langle 11|)/2$. The effective Bell-state describes an ensemble with ϵN molecules in Bell-state $(|00\rangle + |11\rangle)/\sqrt{2}$ and $(1-\epsilon)N/4$ molecules in each of the calculating-basis states $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. According to Ref.[22], it can be decomposed into

$$\rho = \sum_{i,j} \frac{1}{4} \left(\frac{1}{9} + C_{ij} \right) P_i \otimes P_j, \quad (44)$$

where $P_i = (1 + \sigma_i)/2$ for $i = 1, 2, 3$ which represents a pure state polarized along the three axis x , y and z respectively, and $P_i = (1 - \sigma_i)/2$ for $i = 4, 5, 6$ which represents a pure state anti-polarized along the three axis x , y and z respectively. The coefficient C_{ij} are given in Table I. The two different compositions of the effective

Bell-state can be distinguished by observing the fluctuation of the operator

$$\Sigma_{zz} = \sum_i \sigma_{1z}(i) \sigma_{2z}(i). \quad (45)$$

For the ensemble implied by (43), the fluctuation is $(\Delta\Sigma_{zz})_{1,E} = \epsilon\sqrt{N}$, whereas for the product state expansion (44), the fluctuation is $(\Delta\Sigma_{zz})_{2,E} = \frac{2\sqrt{N}}{3}$.

Hence the two ensembles are distinguished though they all have the same compressed density matrix. The decomposition of the effective Bell-state compressed density matrix into a product state compressed density matrix can not be used to infer the conclusion that no entanglement exists in the effective Bell-state. Entanglement is the property of the individual molecules, not the ensemble as a whole. As in Ref.[23], even if all the molecules in an ensemble are in the same quantum state, there is no entanglement between different molecules. Hence the effective pure state should be considered as what it is physically, and there are indeed quantum entanglement within each molecule, though only a small portion of the molecule from the effective pure state contribute to the final read-out in the NMR detection signal.

25. In addition, there is an unnaturalness difficulty in the product state decomposition description of the NMR quantum computing used in Ref.[22]. In the effective pure state NMR quantum computing, the quantum computation is performed on the ϵN molecules in the effective pure state. In the product state decomposition, if only single qubit operations are performed one can still retain a simple picture. We can visualize that there are several "tubes" in the NMR sample. For instance in a two-qubit system case, there are 36 "tubes" in the sample, each tube contains some number of molecules in a product state $P_i \otimes P_j$. A single qubit operation just changes the single molecule state into another state so that one can still use the same "tubes" to describe the state of the ensemble. However once an entangling operation such as the controlled-NOT gate is performed, the number of molecules within each composition, that is in a "tube", will change. For example, if we perform a CNOT gate on effective Bell-state (43), this changes the ensemble into an effective $|+x, 0\rangle$ -state, that is, the first qubit is in $|+x\rangle$ state and the second qubit is in $|0\rangle$ state,

$$\rho_x = \frac{(1-\epsilon)}{4} I_4 + \epsilon | +x, 0\rangle \langle +x, 0|, \quad (46)$$

which is natural and clear. However in the product state expansion of Ref.[22], this density matrix becomes

$$\rho'_x = \sum_{i,j} \frac{1}{4} \left(\frac{1}{9} + C'_{i,j} \right) P_i \times P_j, \quad (47)$$

where the coefficients $C'_{i,j}$ are given in Table II. We see that there is a reshuffling of the number of molecules

	P_1	P_2	P_3	P_4	P_5	P_6
P_1	$\epsilon/3$	$\epsilon/3$	$5\epsilon/3$	$-\epsilon/3$		
P_2			$\epsilon/3$			
P_3			ϵ			
P_4	$-\epsilon/2$	$-\epsilon/3$	$-\epsilon$	$-\epsilon/3$	$-\epsilon/3$	ϵ
P_5			$\epsilon/3$			$-\epsilon/3$
P_6			$\epsilon/3$			$-\epsilon/3$

TABLE II: C'_{ij} for the effective pure state $|+x, 0\rangle$. A space means that coefficient is zero.

in different states. In order to get the same averaged result of the effective $|+x, 0\rangle$ state, one has to reshuffle the distribution of the molecule numbers in different "tubes". While for non-entangling operations, there is no need for such a reshuffling because the single-qubit operation can be performed on each composition of states directly, and their effect is to change state P_i to state $P'_i = UP_iU^\dagger$.

26. One objection to Eq. (36) is that each molecule in an ensemble is in a mixed state itself, even at a given instant.

In this case, the fluctuation of observable Ω is

$$\Delta\Omega_E = \sqrt{N\text{Tr}(\rho\Omega^2) - N(\text{Tr}(\rho\Omega))^2}. \quad (48)$$

In this case, all molecules in the ensemble are equivalent and no physical means can distinguish them. In fact, there is no difference at all, because the compositions of the ensembles are the same. This has been used by some authors to criticize d'Espagnat [24]. To this objection, we stress that it is impossible to prepare such an ensemble using classical probabilities. For instance, in the example given by Peres [3], the state of a photon is prepared according to the result of a coin-tossing, either along z or along $-z$. It is true that each photon has 50% probability to be prepared in state $|0\rangle$ or $|1\rangle$. But each photon is prepared in a definite state, not in a mixed state. This is exactly the case in the BB84 quantum key distribution protocol[13] where the state of a qubit has 25% probability in each of the four states $|z\rangle$, $| - z\rangle$, $|x\rangle$ and $| - x\rangle$. But it is certainly in one of the four possible states.

One possible way to realize such a scenario is that each molecule is in an improper mixed state. For instance in an ensemble of molecules, each molecule contains two qubits A and B , and the two qubits are in an entangled

state, say

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|00\rangle_{AB} + |11\rangle_{AB}). \quad (49)$$

If one looks at the state of the first qubit in each molecule in the ensemble, the resulting state is an improper mixed state. Then in this case, by observing the fluctuations of observables for qubit A alone one can not distinguish another ensemble with the same compressed density matrix where A and B are in state

$$|\psi'_{AB}\rangle = \frac{1}{\sqrt{2}} (|01\rangle_{AB} + |10\rangle_{AB}). \quad (50)$$

However, the above picture is not true in NMR quantum computing. Gershenfeld and Chuang have explicitly explained that in effective pure state there are some numbers of molecules in a definite quantum state[25]. This is a valid approximation for NMR quantum computing because nuclear spins are well isolated from the environment, hence it has a long decoherence time. For those nuclear spins that are not used in quantum computing, decoupling pulses are usually used to disentangle them from the working nuclear spins so that they can not form entangled state that will make the working qubits in an improper mixed state. Thus a valid picture of the ensemble used in NMR quantum computing is that the ensemble contains lots of molecules, there are certain number of molecules in each of the quantum states of the molecule. The spin-relaxation time T_1 can be viewed as the time period a molecule remains at a given quantum state. This is supported by the Gorter formula [26]

$$\frac{1}{T_1} = \frac{1}{2} \frac{\sum_{n,m} W_{n,m} (E_m - E_n)^2}{\sum_n E_n^2}, \quad (51)$$

where $W_{m,n}$ is the transition probability rate from level m to level n . Hence T_1 is the energy weighted time a molecule remain at a given quantum state.

What is then the significance of studying quantum entanglement directly from the density matrix? The study of entanglement for the compressed density matrix directly is of significance because for those compressed density matrices that can not be decomposed into product states, their microscopic entanglement are already reflected in the expectation value. However for ensembles, it is more important to study the entanglement of the pure state of single molecules because it is the place where quantum entanglement exists. As we see, even though the expectation value does not show the entanglement, one can still exploit this precious resource through some method. On the other hand, for improper mixed state, the study of entanglement based on density matrix is of importance.

7. SUPPORTING EXAMPLE FROM QUANTUM COMMUNICATION

27. Though fluctuations of observables in ensembles with infinite number of photons can not distinguish different preparations, there are still methods to distinguish them if one has individual access to the photons in the ensemble. The quantum key distribution is a good example. First we briefly describe the BB84 quantum key distribution scheme[13]. In the BB84 scheme, Alice sends a sequence of photons to Bob. Each photon is randomly in one of the four states: $|0\rangle$, $|1\rangle$, $|+x\rangle$, $|-x\rangle$ respectively. Hence the compressed density matrix of the ensemble, with infinite number of photons theoretically, is $\rho = \frac{1}{2}1_2$. Then Bob chooses randomly one of the two measuring devices, the σ_z -basis or σ_x -basis to measure the state of the photons. After the transmission, Alice and Bob publicly compare their measuring-basis used for each photon, and they retain those events in which they choose the same measuring-basis. From these retained events, they choose a sufficiently large subset of events and publicly compare the measuring results of these events. If the error rate is high, they conclude that there is Eve during the transmission and discard the results. Otherwise they proceed to the post-processing stage and get a final secret key.

If the compressed density matrix had described all the physical properties of the ensemble, we would run into difficulty in the security of quantum key distribution. The same compressed density matrix could also be produced by Alice with only two states $|0\rangle$ and $|1\rangle$: she randomly prepares the photons in one of these two states. In this way, the compressed density matrix is the same $\rho = \frac{1}{2}1_2$. Immediately we know that this replacement is invalid: the simplified scheme is unsafe, for if Eve uses the σ_z measuring device to measure every photon, she can steal every bit of information. Then she can resends a photon with the same state to Bob. In this way, her action could not at all be detected. Hence the scheme becomes insecure. This conclusion would not alter if we had used infinite number of photons in the ensemble.

8. SUMMARY

28. We have examined in details the definition of ensembles in quantum mechanics and the different definitions of mixed states. We have proposed to use different terminologies for the density matrix in different situations: the full density matrix, the compressed density matrix and the reduced density matrix. We have explicitly shown that ensembles having the same compressed density matrix but different compositions can be distinguished physically by observing fluctuations of observables in the whole ensemble. With this conclusion at our hand,

we studied the problem of the nature of NMR quantum computing. We have pointed out that the conclusion that there is no entanglement in the current NMR quantum computing experiment is based on an unjustified belief that ensembles having the same compressed density matrix are physically equivalent. This conclusion is also supported by the security aspect of quantum key distribution where the density matrix ρ could not specify all the physical properties of an ensemble, even if the number of molecules in the ensemble is infinite. A brief summary is given in Table III.

GLL are grateful to Professors C. N. Yang, Alain Aspect, Peter Zoller, Hans Briegel, Li You, C P Sun, K. N. Huang, Brian J Dalton for helpful discussions. They also thank X. B. Wang, Minki Jeong, Piero Mana for email discussions. HWL is supported by a grant from the Korea Science and Engineering Foundation (KOSEF) through Korea-China International Cooperative Research Program. This work is supported by the National Fundamental Research Program Grant No. 001CB309308, China National Natural Science Foundation Grant No. 10325521, 60433050, the Hang-Tian Science Fund, and the SRFDP program of Education Ministry of China.

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TABLE III: A summary

Full density matrix	
Object described	A single quantum system, but may contain many molecules
Matrix Name	Full density matrix $\rho_f = \psi\rangle\langle\psi $
Object Name	A pure state. The object is always described by a single wave function, or equivalently a full density matrix for a pure state
Remark	The description is complete. Different preparations with the same full density matrix are physically identical.
Compressed density matrix	
Object described	An ensemble of N independent molecules with N_i molecules in state $ \psi_i\rangle$.
Matrix Name	Compressed density matrix $\rho_c = \sum_i \frac{N_i}{N} \psi_i\rangle\langle\psi_i $. ρ_c describes the state of an averaged molecule from this ensemble. The full density of the whole ensemble is $\rho_f = \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_N$, where the state of different molecules can be the same. Though two molecules may be in the same quantum state, they are distinguishable, for instance by their positions in space. The relation between the full density matrix and the compressed density matrix is $\rho_c = \frac{1}{N} \sum_i \rho_i$, where ρ_i is the full density matrix for molecule i in the ensemble.
Object Name	The object described by ρ_c is called a proper mixture.
Remarks	One can not tell the difference between two ensembles having the same compressed density matrix by sampling measurement or by the average value, but they can be distinguished by observing the fluctuations of observables regarding the whole ensemble.
Reduced density matrix	
Object described	Composite quantum systems
Matrix Name	Reduced density matrix which is obtained by taking trace over other degrees of freedom from the full density matrix of the whole composite system.
Object Name	improper mixture.
Remark	By observing the observables of only a part from the composite system, it is impossible to distinguish systems with the same reduced density matrix. But the composite systems can be distinguished if the whole composite systems are measured.